

state-of-the-art molecular modeling techniques can be used to study complicated macromolecular complexes, whose structures have not yet been experimentally determined, and to validate these against the available experimental data. The proposed structure will facilitate future studies on the rational design of successful Aflatoxin B1 (AFB1) modulators or on human subpopulations characterized by specific CYP3A4 polymorphisms that are especially sensitive to AFB1 - the most potent natural carcinogen known to men. We also report a series of ab initio and density functional theory simulations of guanine alkylation by aflatoxin B1 exo-8,9-epoxide and predict that the preference of aflatoxin B1 exo-8,9-epoxide over the endo stereoisomer for the reaction with guanine exists in the aqueous solution and is only further amplified in the DNA duplex. Finally, through comparison with an analogous reaction between 3a, 6a-dihydrofuro[2,3-b]furan exo-4,5-epoxide and guanine, we show that the large planar body of aflatoxin B1 does not enhance its reactivity and related carcinogenicity. This explains why the planar region of related mycotoxins sterigmatocystin and aflatoxin G1 could have been evolutionarily optimized in a different way.

T.4.3.2 – Simulation of the UV-vis Spectra of Flavonoids - Jelena Tosovic, Zarko Milosevic and Svetlana Markovic

The UV/Vis properties of 14 naturally occurring flavonoids, including flavones, flavonols, and isoflavones, were investigated. The TDDFT approach in combination with the B3LYP method and 6-311+G(d,p) basis set was applied. To avoid the Kohn-Sham orbitals, whose shapes are misleading when used to interpret and describe electronic transitions, the natural bond orbital analysis was applied. Taking into account the energy gap, spatial separation, and character of the π bonding, lone pair, and π^* antibonding natural localized molecular orbitals (NLMOs), the "NLMO clusters" were constructed. NLMO cluster is a molecular moiety characterized with distinguished electron density. Our investigation showed that the TDDFT and NBO approaches are complementary, implying that the results from the two theories can be combined to better understand the redistribution of electron density upon excitation. Agreement between the predictions of the TDDFT approach and those based on the NLMO clusters is excellent in the case of major electronic transitions and small excitation energies.

T.4.3.3 – DFT Investigation of the Reaction Cyanidin with Hydroxyl Radical - Dejan Milenkovic, Jasmina Dimitric Markovic and Zoran Markovic

Cyanidin, as one important plant pigment, was theoretically (at M05-2X/6-311+G(d,p) level of theory) investigated for its ability to scavenge potentially highly damaging hydroxyl radical. The applied method successfully reproduces the bond dissociation enthalpy (BDE), the ionization potential (IP) and proton affinity

(PA). The HAT mechanism is most favorable reaction pathway for antioxidative action of cyanidin in the gas phase. On the other hand, the SPLET mechanism is the most favorable reaction pathway for antioxidative action of cyanidin in the aqueous phase. Mechanistic investigations of antioxidative action of cyanidin in reaction with the hydroxyl radical confirmed that HAT is the dominant reaction pathway in the gas phase, and that the 4' position is the most reactive.

T.4.3.4 – Some Examples on the Performance of Density Functional Theory in the Description of Bioinorganic Systems and Processes - Tiziana Marino, Nino Russo, Emilia Sicilia and Marirosa Toscano

Density functional computations on a series of complex systems and processes are presented and discussed. In particular, the following subjects have been investigated: i) catalytic mechanism of carbonic anhydrase; ii) structural properties of silver mediated DNA dimers; iii) structural and spectroscopic features of Zn-phthalocyanine derivatives; iv) carnosine-carboplatin, carnosine-oxaliplatin complexes fragmentation pathways. Reported data indicate that good results can be obtained selecting the appropriate computational strategies, exchange-correlation functionals and basis sets.

Session T.5.1 - Pacific room: 17:00-18:30 Biomedical Signal Processing (part II)

Chair: Dimitris Fotiadis

T.5.1.1 – An Unsupervised Methodology for the Detection of Epileptic Seizures in Long-term EEG Signals - Kostas M. Tsiouris, Spiros Konitsiotis, Sofia Markoula, Dimitrios D. Koutsouris, Antonis I. Sakellarios, and Dimitrios I. Fotiadis

An unsupervised methodology for the detection of Epileptic seizures in EEG recordings is proposed. The time-frequency content of the EEG signals is extracted using the Short Time Fourier Transform. The analysis focuses on the EEG energy distribution among the well-established delta, theta and alpha rhythms (2-13 Hz), as energy variations in these frequency bands are widely associated with seizure activity. Relying on seizure rhythmicity, the classification is performed by isolating the segments where each rhythm is more clearly and dominantly expressed over the others. For the first time, an unsupervised methodology is evaluated using more than 978 hours of EEG recordings from a public database. The results show that the proposed methodology achieves high seizure detection sensitivity with significantly reduced human intervention.

T.5.1.2 – Walsh-Hadamard Spectral Analysis of Signals Representing Bioelectrical Activity of the Reproductive Tract in Pigs - Edward Oczeretko, Marta Borowska, Ewelina Brzozowska, Bartosz Pawlinski, Andrzej